

## ProtoADME

ProtoADME is a computational (*in silico*) tool focused on the prediction of endpoints related with the ADME (Absorption, Distribution, Metabolism and Excretion) of chemical substances.

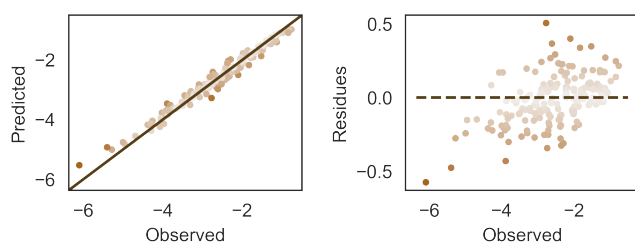
## Endpoint

### Toxicokinetic: skin permeability

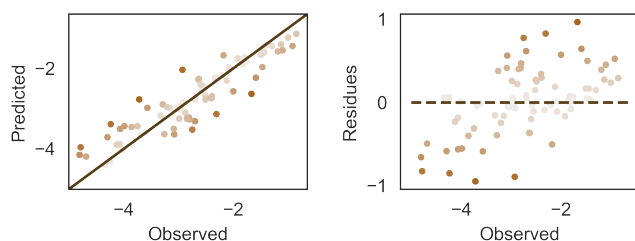
Skin permeability is a measure of the absorption of a compound through the outer surface of the skin.

## Metrics

### Training set



### Validation set



Parameters	Training	Validation
$R^2$ score	0.97	0.84
Mean absolute error (MAE)	0.13	0.30
Mean squared error (MSE)	0.03	0.16
Median absolute error	0.09	0.24
Explained variance	0.97	0.84

ProtoADME is part of



ProtoPRED platform allows the easy, fast and user-friendly prediction of different properties of chemical compounds, using proprietary (Q)SAR models.

+34 962 021 811

protopred@protoqsar.com

<https://protopred.protoqsar.com/>

© 2024 ProtoQSAR, S.L.